Anthocyanin degradation of *Hibiscus sabdariffa* extracts during storage monitored by MCR-ALS on UV-VIS spectra

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Calyces of *Hibiscus sabdariffa* are traditionally used to prepare a red beverage rich in anthocyanins (delphinidin- and cyanidin-3-O-sambubioside) by decoction in water. These molecules are subjected to degradation during storage leading to a undesirable color intensity decay and change from red to brown in few months. The chemical origins of this quality loss have been already identified as scission and mainly condensation reactions leading to uncolored or brown polymers of anthocyanins (Sinela et al., 2016). Scission and condensed products are known to be instable and/or of various molecular weight. Their concentration is therefore very difficult to get unless numerous time- and money-consuming analysis. An alternative of getting mecanistic and kinetic insigth into anthocyanin degradation during processing or storage is the UV-VIS spectra analysis with chemometric tools. Indeed, UV-VIS spectra are easy to get, but may be complex to interpret as they result from the contribution of all molecules that absorb in this spectral region, which is the case of most of the polyphenols.

The objective of this study is to use spectral deconvolution by mean of Multivariate Curve Resolution-Alternating Least Squares (MCR-ALS) on spectral evolution of *Hibiscus sabdariffa* extract obtained by soaking calyx powder in water at a ratio 1/9 (g/g) during one month of storage at 37°C. In this work, we propose a two-steps approach: a first deconvolution on two fractions of the extract, low molecular and high molecular weigth fractions obtained by size-exclusion chromatography and a MCR done on the spectrum of the whole extract. Absorbance from 250 to 700 nm (each 0.5 nm) was recorded on 10 samples at different storage times. MCR-ALS was carried out on the 10 spectra using a toolbox developped by Jaumot et al. (2005) on Matlab (The MathWorks, Inc., Natick, MA, USA) with a non negativity constraint algorithm. To improve the mathematical resolution and the chemical validity, the data set was augmented with pure spectra obtained with standards in solution.

The results showed that the deconvolution made on the fractions obtained with size-exclusion chromatography was useful to extract qualitative information in the form of spectra of the low and high molecular weigth compounds. Three spectra were clearly identified as anthocyanin (with a spectral contribution equivalent to their relative concentration), chlorogenic acid, scission products (gallic and protocatechuic acids) and two spectra were attributed to condensed molecules (because of their absorbance in the brown region) and other colorless anthocyanin forms in equilibium (because of their peak in the UV region). The five spectra were used to improve the MCR-ALS applied to the whole extract. For this second step, the relative concentration of each specy was obtained. The anthocyanin evolution could be modeled by a first-order kinetic with a rate value consistent with litterature. Chlorogenic, gallic and protocatechiuc acids were found stable as expected. A significant evolution was evidenced for condensed molecules whose relative concentration increased by a 1.6-fold.

To conclude, MCR results on *Hibiscus sabdariffa* extracts, fractionnated and not, were interesting since they could successfully represent the evolution trend of the different species in solution during storage: the anthocyanin but also their degradation products.

Keywords: delphinidin; cyanidin; phenolics; MCR-ALS; UV-VIS spectra

References

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Book of Abstracts

2-4 November 2016, Barcelona / Spain

THE FOOD FACTOR I
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INTRODUCTION

This book contains a selection of the abstracts that were accepted for presentation at The Food Factor I Barcelona Conference, Established, emerging and exploratory food science and technology, which was held at the University of Barcelona, Spain, from 2 to 4 November 2016.

The first edition of this Food Factor Conference gathered around 250 participants, coming from more than 45 countries. And around 280 works were presented at the conference. This was a more than satisfactory level of attendance for this first research forum, especially in the context of a global budget constraint.

The organization called for research papers dealing with the following topics:

Food chemistry and biochemistry
Topics: structure and function of major and minor components (either nutrient or non-nutrient) of foods, the biochemical changes produced during handling, storage, post-harvest/mortem processing, distribution or due to domestic conditions, and their impact on nutritional, physiological, sensorial, or toxicological properties and safety; Reports on new or improved techniques or methods for addressing these topics or on the chemistry of food contacting materials. Specific areas of interest were:

- Food bioactives
- Chemistry of food additives and preservatives
- Chemical analysis for the determination of authenticity and origin of foods
- Biochemical changes in cereal grains and legumes due to postharvest conditions and treatments (storage, germination, fermentation…)
- Biochemical changes in postharvest fruits and vegetables with impact in quality
- Biochemical changes produced in the conversion of muscle into meat and fish
- Biochemistry of the biosynthesis of milk components
- Biochemical changes of the transformation of milk into dairy products
- Browning reactions in foods
- Lipid peroxidation
- Computational chemistry in food research
- Chemistry of food packaging and food-handling materials

Food microbiology
Topics: microorganisms that are related to human nutrition and health: those used to make foods or whose use and/or consumption can improve food production or host health; the detection, identification and quantification of those that pose a threat to food safety or quality (also applied to microbial toxins and metabolites and foodborne viruses); the study of their biology (biochemistry, ecology, genetics, physiology…); their role in various food processing methods and in food spoilage; their susceptibility to different physical or chemical agents, processing or packaging methods; or their interaction with different food chain environments and foodstuff, reports on the development and application of mathematical and computational tools in food research . Specific areas of interest were:

- Rapid detection of foodborne pathogens
- High throughput screening
- Norovirus and other viral agents in foods
- Antimicrobial/biocide resistance
- Microbial risk analysis: assessment, management and communication
- Microbiology of fermented foods and beverages
- Food defense

- Food contamination
- Mycotoxins
- Intestinal microbiota and host health
- Hygienic design of food manufacturing lines
- Epidemiology of foodborne pathogens
- Spoilage of soft drinks (with increasing levels of nutrients)
- Biofilms
- Cross-contamination
- Beneficial microbes
- Food parasites
- Microbial nutrition: probiotics
- Bacterial and fungal species: *Yersinia, Bacillus, Staphylococcus, Listeria, Salmonella, Escherichia coli, Vibrio, Campylobacter, Brucella, Mycobacterium, Clostridium, Streptococcus*, and others; Aflatoxins and other microbial-derived toxins; Norovirus, Rotavirus, Hepatitis virus and other viral agents

Food physics
Topics: understanding and measurement of the physical properties of foods and their constituents: structural, rheological, textural, optical, electrical, thermodynamic, flowing, acoustic, mechanical…, how they change during processing, the relationship between the properties of their constituents (water, proteins, fats, oils, gasses, and minor constituents like vitamins and minerals) and their macroscopic properties (texture, taste, smell, colour, nutritional and health impact), or the developments of purely physical ways of treating foods, either thermal or non-thermal. Specific areas of interest are:

- Thermal modification of foods: heat-moisture treatment, annealing, microwave heating, osmotic pressure treatment …
- Non-thermal modification of foods: ultrahigh-pressure treatments, instantaneous controlled pressure drop, high-pressure homogenizers, dynamic pulsed pressure, pulsed electric fields, freezing, thawing…
- Multiscale computer simulation and mathematical modeling of food structures
- Novel microscopy, image analysis, and characterization techniques
- Soft matter physics applied to food materials
- Colloidal structures, their interactions and relationship with food stability and overall macroscopic properties
- Modern technologies for sensory analysis
- Relationship between physical properties of food and consumer preferences

Food analysis
Topics: analysis of foods and their constituents (amino acids, peptides, proteins, phenolic compounds, carbohydrates, DNA fragments, vitamins, functional ingredients or nutraceuticals, toxins, pesticide and drug residues, industrial, processing and packaging contaminants, additives, allergens, antibiotics, nanoparticles,…) by the use of analytical and imaging techniques and methods, in the context of the assessment of food structure, quality, safety, traceability, origin, authenticity, health benefits of certain constituents…; works featuring the analysis of large amounts of data generated by different techniques or time series of many variables (chemometrics). Specific areas of interest were:

- Instrumental techniques: biological, separation, spectroscopic, rheological, thermal, radiochemical, electrochemical, miniaturized microfluidic systems, modern foodomics and/or systems biological approaches…
- Imaging techniques: optical, confocal, electron, atomic force microscopies…
- Analysis of sensory properties of foods

- Sample preparation
- Qualitative analysis in a chemometric context
- Data pre-processing
- Calibration standards
- Hyperspectral images
- Image analysis and processing in food science and in industry
- Ingredient distribution in products
- Microstructures of foods: characterization and distribution
- e-noses and e-tongues
- Consumer behaviour

Food processing and packaging
Topics: established and novel processing and packaging technologies applied for delivering foods that last longer before spoiling (preservation), and that are available, safe, nutritious, and convenient, while minimizing environmental impact. Specific areas of interest were:

- Active and intelligent packaging
- Migration and potential health effects of packaging-associated chemicals of concern (Bisphenol-A, semicarbazide…)
- Modified atmosphere packaging
- Established and modern processing and preservation technologies: drying, cooling, freezing, heating, salting, fermentation, pasteurization, additives addition, irradiation, hurdle technology, use of high-pressure and pulsed electric field processing, dense phase carbon dioxide, ozone, ultrasonics, cold plasma, IR technologies, natural antimicrobials, oxygen depleted storage, microwave heating, low shear extrusion…
- Green technologies: supercritical fluid extraction, membrane technology, bioconversions…
- Biorefinery in the production of food components (proteins, carbohydrates, fats…)
- Dietary, health, and environmental concerns related to food processing
- Waste reduction in food processing and valorization of by-products

Food engineering and hygienic design
Topics: (hygienic) design and (safe) operation of food plants, including engineering tools for assessing and managing risks. Specific areas of interest were:

- Heat, mass transfer and fluid flow in food processing
- Artificial intelligence in food research and industry
- Mathematical modelling and software development for food research and industry
- Finding, correcting and preventing hazards in food industry: Hazard Analysis and Critical Control Point (HACCP), Microbial Risk Assessment (MRA)…

Environmental impact of food production and consumption
Topics: environmental impact of the food supply chain (carbon and water footprint, biodiversity, land use...), for each of the food groups. Specific areas of interest were:

- Food waste impact on climate, water, land and biodiversity
- Ways of reducing environmental impact
- Environmental impact of meat production

Foods of plant origin
Topics: plant, animal, crop or soil science relevant to the production of foods of plant origin: cereals, legumes, fruit and vegetables, sugar crops. Specific areas of interest were:

- Understanding phytobiomes for improved crop productivity
- Farming animal science: cattle, sheep, goats, horses, pigs, poultry
- Soil science

- Sustainable farming systems
- Genetic and non-genetic crop improvement
- Plant and crop protection
- Crop models
- Improvement of water use
- Resistance to pests and disease
- Modification of crops for reducing waste
- Filling the gap between plant and crop physiology
- Stress in crops produced by changing environmental conditions

Foods of animal origin
Topics: animal, vegetal, soil or marine/aquatic science relevant in the production of foods of animal origin: meat, fish, milk and their derived products, eggs, insects...

The regular conference program was complemented with two Plenary Lectures:

"Highlighting natural value: physical and chemical approaches in food processing" by Isabel C.F.R. Ferreira, from the Mountain Research Centre (CIMO), ESA, Polytechnic Institute of Bragança, Portugal

"Nonthermal processing technologies for food: Current applications and future perspectives" by Pedro Elez-Martínez, from the University of Lleida, Spain

We hope attendants and readers in general will find the content of this book of abstracts interesting, inspiring and useful and we look forward to seeing you in another fruitful edition of the conference in 2018.

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